Free cooling and inelastic collapse of granular gases in high dimensions

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(February 1, 2008)

The connection between granular gases and sticky gases has recently been considered, leading to the conjecture that inelastic collapse is avoided for space dimensions higher than 4. We report Molecular Dynamics simulations of hard inelastic spheres in dimensions 4, 5 and 6. The evolution of the granular medium is monitored throughout the cooling process. The behaviour is found to be very similar to that of a two-dimensional system, with a shearing-like instability of the velocity field and inelastic collapse when collisions are inelastic enough, showing that the connection with sticky gases needs to be revised.

PACS numbers: 47.50.+d, 05.20.Dd, 51.10.+y, 47.11.+j

An important difference between a molecular fluid and a gas of mesoscopic or macroscopic grains is the possibility for the latter, associated with the inelastic nature of the collisions, to exhibit clustering and collapse [1–3]. A large and rapidly growing body of theoretical work is devoted to clustering, which consists in a long wavelength low frequency hydrodynamic phenomenon, and refers to the formation of density inhomogeneities. On the other hand, the phenomenon of inelastic collapse, which is a short wavelength and high frequency singularity inherent to the inelastic hard sphere (IHS) model, seems much less understood, except in one dimension [4].

In the IHS model, grains are modeled as smooth hard spheres undergoing binary, inelastic and momentum-conserving collisions, which dissipate a constant fraction $(1-r)$ of the component of the relative velocity $\mathbf{v}_{12}$ along the center-to-center direction $\hat{\boldsymbol{\sigma}}$. Noting with primes the post-collision velocities, this translates into $\mathbf{v}'_{12}\cdot\hat{\boldsymbol{\sigma}} = -r\,\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}}$, while the tangential relative velocity (perpendicular to $\hat{\boldsymbol{\sigma}}$) is conserved.

In an interesting article, Ben-Naim *et al.* proposed that a freely evolving inelastic gas belongs asymptotically to the universality class of the sticky gas [5], for which $\mathbf{v}'_{12} = \mathbf{0}$ after each collision. Noticing that the temperature T of an inelastic gas is a monotonically increasing function of the restitution coefficient r and therefore bounded from below by the totally inelastic case ($r = 0$), these authors invoked a mapping onto Burgers' equation to conjecture that the inelastic collapse is avoided for space dimensions $d > d_c = 4$, and that the standard Haff's cooling law $T \propto (\epsilon t)^{-2}$ where $\epsilon = (1-r^2)/(2d)$, holds indefinitely above this critical dimension d_c. Velocity fluctuations and scaling exponents in one dimension can indeed be described by the inviscid Burgers equation [5]. However, in higher dimensions, the completely inelastic version of the IHS model, with $r = 0$, does not strictly correspond to the sticky gas limit because the tangential relative velocity is not dissipated in a binary encounter ($\mathbf{v}'_{12}\cdot\hat{\boldsymbol{\sigma}} = \mathbf{0}$, but a priori $\mathbf{v}'_{12} \neq \mathbf{0}$), so that it is interesting to test the validity of the above-mentioned predictions. In this article, we report Molecular Dynamics (MD) simulations of IHS gases for $d = 4, 5$ and 6. For each space dimension, the relevant parameters ϕ (packing fraction) and r (normal restitution) are varied for systems consisting typically of $N = 5.10^3$ to 5.10^4 particles. The code was first successfully tested by comparing for various densities the MD equation of state (or equivalently the pair correlation function at contact) with the analytical approximation of Song *et al* [6]. For all investigated dimensions and for high enough dissipation ($r \leq 0.2$ for $d = 5$ and $r \leq 0.1$ for $d = 6$), the system exhibits the finite time singularity characteristic of the inelastic collapse, in contradistinction to the conjecture of [5], with a situation closely reminiscent to its two dimensional counterpart [2]: the (hyper)spheres collide infinitely often in a finite time along their joint line of centers. Following Refs. [2] we probed this multi-particle process occurring through the accumulation of an infinite sequence of binary collisions by a contact criterion: after each collision, the relative distance d^* between the next two colliding partners is monitored; if this interparticle spacing normalized by the diameter σ has decreased and becomes of the order of machine precision, a three body interaction has occurred, corresponding to an inelastic collapse. The results of a typical run ($d = 5$) are shown in Fig. 1. When a multi-body interaction commences, d^* decreases geometrically with the number of collisions, as in two dimensions [2]. Enforcing a high precision computation allows to follow the decay over more than 26 orders of magnitude (whereas only 8 orders are accessible with a standard double precision algorithm, see the inset of Fig. 1). After a collapse has occurred, the inaccuracy of the computer disperses the collapsing cluster, before another multi-body event involving different

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particles occurs at a different location. Our analysis indicates that on a hypothetical infinite precision machine, the collapse would continue forever whereas roundoff errors act as an effective regularization. Throughout a collapse, the time between two successive collisions follows a geometrical decrease very similar to that displayed in Fig. 1.

Let us note that the seemingly low value of the packing fraction ϕ in Fig. 1 is a misleading effect of "high" dimensionality. It turns that the reduced density

$$n^* = n\,\sigma^d = \frac{d\,2^{d-1}}{\pi^{d/2}}\,\Gamma\left(\frac{d}{2}\right)\phi \tag{1}$$

where n is the number density and Γ the Euler function, is a more relevant parameter to discriminate between "low" and "high" densities. In a simple cubic lattice, the highest packing achievable with spheres at contact corresponds to $n^* = 1$. The configuration of Fig. 1 with $\phi = 0.08$ corresponds to $n^* = 0.5$ and is consequently of high density. We considered the possibility that the conjecture of [5] applies in the opposite limit of low packing (that would correspond to the so called sticky dust in the case of vanishing both normal and tangential restitution coefficients). We lowered ϕ by an order of magnitude which requires to consider large systems to avoid a spurious increase of the mean free path; our simulations with $N = 2.10^5$ particles and $\phi = 0.008$ ($n^* = 0.05$) in five dimensions nevertheless exhibit inelastic collapse for $r < 0.05$.

When the restitution coefficient is above a critical threshold, the inelastic singularity is absent and we can follow the time evolution of the system. Initial conditions for all inelastic runs were equilibrated fluid configurations of elastic hard spheres at the corresponding (uniform) density, with a uniform temperature (coarse-grained kinetic energy) and Gaussian distribution of velocities. The short time regime is then given by the homogeneous cooling state, which is essentially an adiabatically changing equilibrium state where the mean kinetic energy E (related to the temperature T by $E = dT/2$ due to the vanishing of the flow field) is given by

$$E(t) = \frac{E_0}{\left(1+\epsilon t/t_0\right)^2}. \tag{2}$$

In Eq. (2), t_0 is the Enskog mean collision time of elastic particles at the same density [7,8] and the inelasticity parameter $\epsilon = (1-r^2)/(2d)$ follows from the assumption of a Gaussian velocity distribution. It has been shown within the framework of Enskog-Boltzmann equation that the corrections due to non Gaussian behaviour on the cooling rate are small for all inelasticities [9]. The internal clock of the system can be parameterized by τ, the average number of collisions suffered per particle in a time t, which reads in the homogeneous cooling state

$$\tau = \frac{1}{\epsilon}\,\ln\left(1+\epsilon\,\frac{t}{t_0}\right). \tag{3}$$

Denoting N_c the total number of collisions having occurred in the system over a time t, we have $\tau = 2N_c/N$. Figure 2 shows that the law $E(\tau) = E_0 \exp(-2\epsilon\tau)$ expected from Eqs. (2) and (3) is only valid at short times. A crossover, indicated in Fig. 2 by an arrow, is generically observed for all runs in dimensions 5 and 6, provided the inelastic collapse is avoided; the crossover time depends both on the inelasticity and on system sizes. After the crossover, the behaviour of E with the number of collisions also depends on system size (see Fig. 3), and $[\ln(E/E_0)]/\tau$ does not scale with the inelasticity as ϵ (inset of Fig. 3). Moreover, Fig. 4 shows that the energy decays like t^{-2}, as predicted in [5]; however, Fig. 4 shows that the prefactor is different at short and large times[1], and (at large times) strongly increases with increasing number of particles; it neither scales with inelasticity as ϵ^{-2} (not shown). All these results are at variance with the suggestions of [5]: the energy at large times decays as $A(N,\epsilon)\epsilon^{-2}t^{-2}$, and not simply as $\epsilon^{-2}t^{-2}$ (Haff's law).

Before reaching the crossover time t_c, the velocity distribution of the particles is isotropic and very close to a Maxwellian. Once the crossover time is elapsed, we observe an evolution reminiscent of the shearing instability found in lower dimensions [1,2,8,10]. Fig. 5 shows the distribution of the components of the rescaled velocity $\mathbf{c} = \mathbf{v}/\sqrt{T(t)}$ for $t \gg t_c$. For the particular system of Fig. 5, two components are found to be Gaussian (the central peaks) and the remaining directions appear as bimodal and concentrate most of the energy. The corresponding shear bands

[1] We note that from Eq. (2), the slope of the dotted line in Fig. 4 (short time behaviour) corresponds to the ratio t_b/t_0 of Boltzmann over Enskog mean collision times, and is an indirect measure of the pair correlation function at contact χ [7]. From Fig. 4, we get $\chi \simeq 1.7$ while the equation of state of Ref. [6] yields 1.74 for the density considered. This value is corroborated by an independent elastic run where we measure $\chi \simeq 1.7$.

are difficult to visualize, but insight can be gained by a suitable projection onto a two-dimensional surface. Such a projection is displayed in Fig. 6. The coherent motion we observe in Fig. 6 suggests that the large time dynamics of the system is controlled by the periodic boundary conditions used in the simulations, as analyzed in [10].

Since, in a 5 dimensional system of 5.10^4 particles, with packing fraction 0.08, the simulation box length L is only 10 times as large as the spheres' diameter, the systems considered here can be considered as small (in the sense that there exists no possible separation of length scales). The behaviour reported here for $E(t)$ is therefore consistent with the two dimensional simulations of Orza *et al.* [12], showing $E \propto A(N,\epsilon)\, t^{-2}$ for small systems, with a prefactor much larger than predicted by Haff's law. Gaining one order of magnitude for L/σ would require to increase N by d orders of magnitude, which is unachievable for $d > 4$. The validity of Brito and Ernst's theoretical prediction for large systems $E \propto \tau^{-d/2}$ [11] (coinciding with the approach of [5] for $d \leq 4$) can consequently not be tested in dimensions higher than 4.

In conclusion, our simulations show the existence of an inelastic collapse in high dimensions, not only for dense systems but also for more dilute ones (even if the situation of very low packing fraction cannot be reached, so that the "sticky dust" limit cannot be tested by numerical simulations). They indicate therefore that the relationship between inelastic and sticky gases put forward in [5] needs to be refined.

It is a pleasure to thank M. Ernst for his continued interest in our work.

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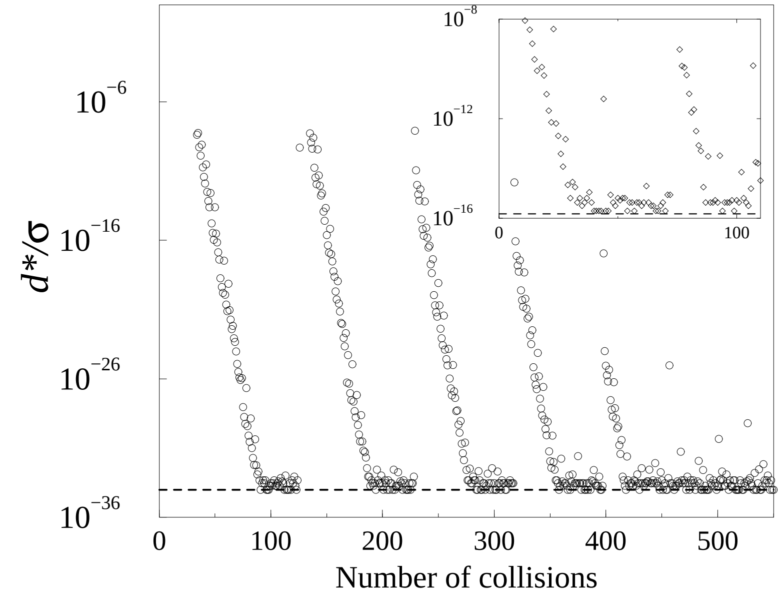

FIG. 1. Normalized inter-particle separation (see text for definition) as a function of the number of collisions since an arbitrary time origin, for $d = 5$, $N = 16807$, $\phi = 0.08$ and $r = 0.1$. Each circle corresponds to a collision and the data were obtained specifying a "quadruple precision" computation (with reals coded on 16 bytes). Each decrease (from 10^{-8} to 10^{-36}) corresponds to repeated collisions between a small number of particles, typically three particles, one bouncing back and forth between two others, with a diverging frequency. For the same system, the inset shows with diamonds the results of a standard "double precision" run (reals on 8 bytes). In both cases, the floor of machine precision is indicated by a dashed line (approximately 10^{-34} for real$\star$16 and 10^{-16} for real$\star$8). Only those collisions with $d^* < 10^{-8}\sigma$ have been displayed.

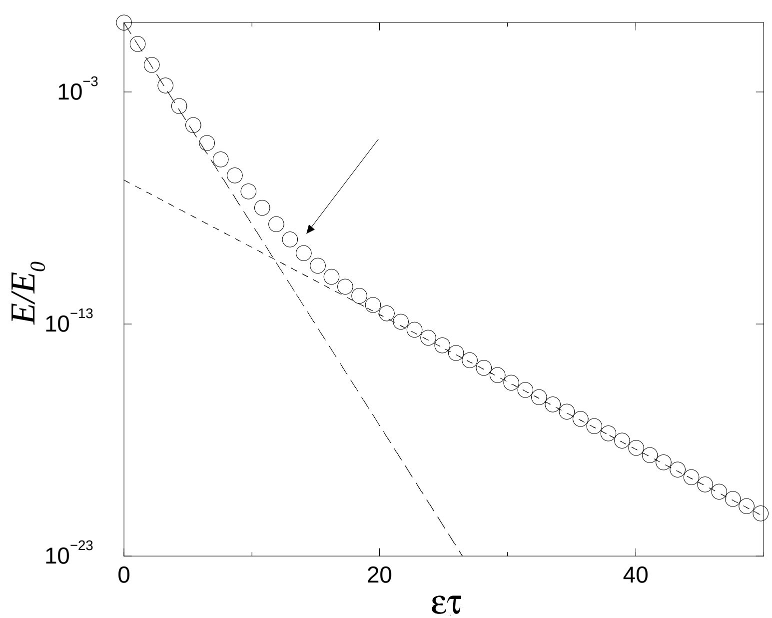

FIG. 2. Evolution on a linear-log scale of the mean kinetic energy (rescaled by its initial value) with the number of collisions per particle for $N = 16807$, $r = 0.6$ ($\epsilon = 0.064$), $\phi = 0.08$ and $d = 5$. The long-dashed line has a slope -2 (Haff's law) while the short-dashed one is a fit to the long time behaviour with slope -0.66.

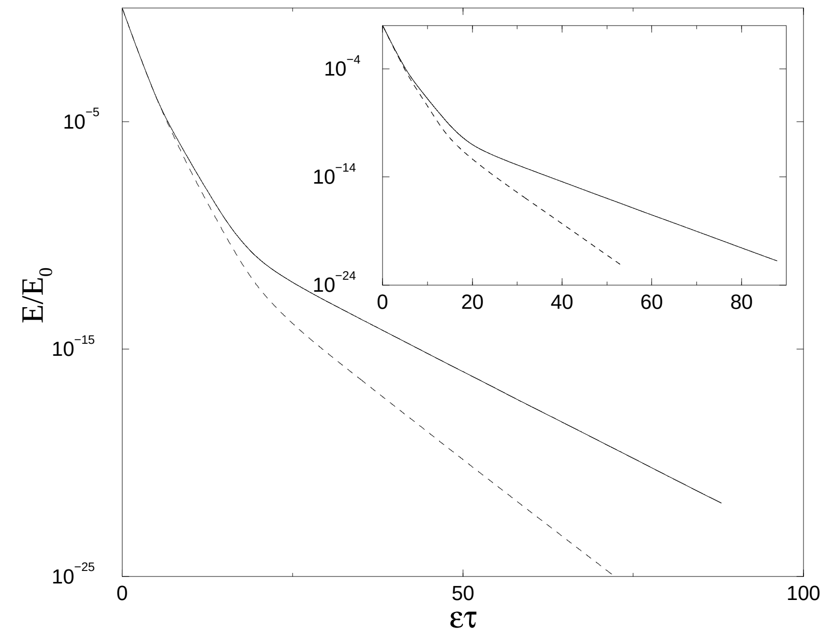

FIG. 3. Linear-log plot of energy versus number of collisions for $r = 0.4$ ($\epsilon = 0.084$), $\phi = 0.08$, $d = 5$ and two system sizes : $N = 16807$ (full curve) and $N = 7776$ (dashed line). The inset shows the dependence with inelasticity for $N = 16807$: $r = 0.4$ ($\epsilon = 0.084$), full curve, and $r = 0.6$ ($\epsilon = 0.064$), dashed line. The energy decay thus depends on the system size and is not only a function of $\epsilon\tau$, as suggested in [5].

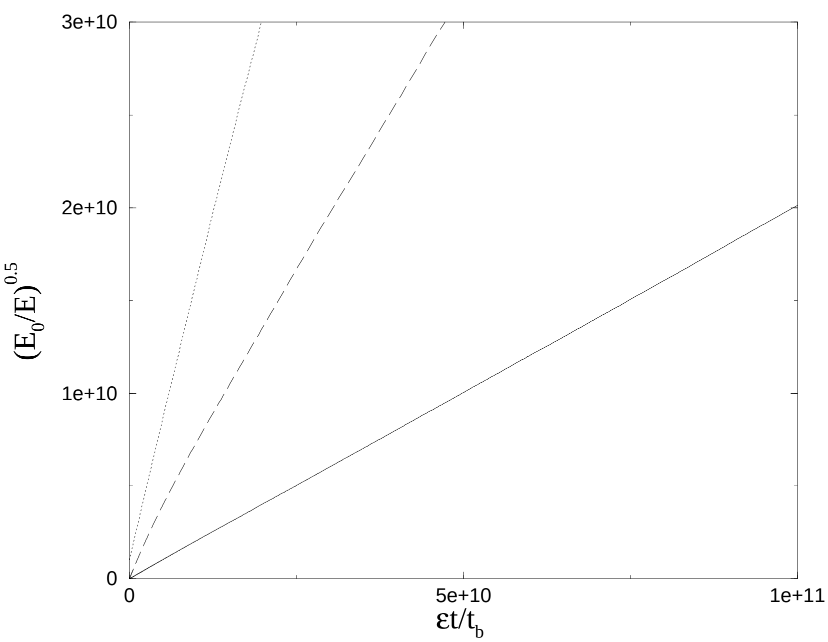

FIG. 4. Time dependence of $\sqrt{E_0/E}$ for $r = 0.5$ ($\epsilon = 0.075$) and $d = 5$. The full and long-dashed curves correspond to the large time behaviour for $N = 16807$ and $N = 7776$ respectively. The dotted line with slope 1.7 is a magnification of the short time evolution, independent of N and ϵ (since the evolution follows Haff's law) obtained by rescaling both x and y axis by the same (large) factor. In the x axis, t is expressed in units of t_b/ϵ where t_b is the Boltzmann mean collision time of elastic particles at the same packing fraction ($\phi = 0.08$). These curves show that, although $\sqrt{E_0/E}$ increases like $\epsilon t/t_b$, the prefactors at short and large times differ, and depend at large times on N and ϵ.

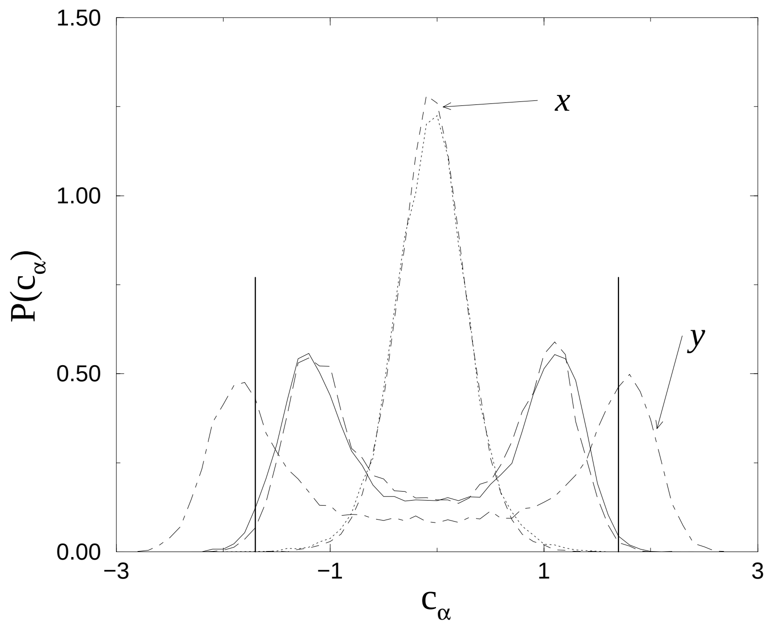

FIG. 5. Probability density distribution of the five components of the rescaled velocity, for $N = 7776$, $r = 0.6$, $d = 5$ and $\tau = 122$. One of the central Gaussian directions is arbitrarily chosen as the x direction and that containing the most significant fraction of the kinetic energy is labeled y. The vertical lines at $c_\alpha = \pm 1.7$ indicate the cutoffs used in the projection scheme producing Fig 6.

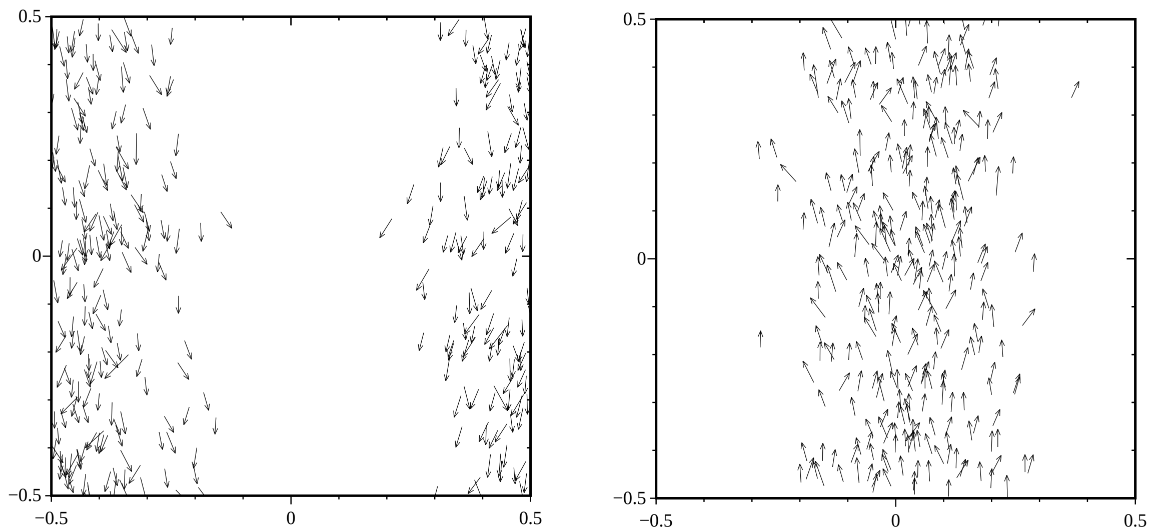

FIG. 6. Projection of the velocities onto the x-y plane, for the same system as in Fig. 5. Only those particles with $c_y < -1.7$ (resp. $c_y > 1.7$) have been shown on the left (resp. right) plot. The simulation box is a cube $[-0.5, 0.5]^5$.